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FINAL REPORT

SIMULATIONS OF TRIBOLOGY AT CARBON/METAL INTERFACES

by

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Objective:

The goal of the project is to gain an increased understanding of the atomic-scale chemical interactions responsible for macroscopic friction and wear when two surfaces are brought into sliding contact with each other. Such insight is crucial to the development of improved solid-state lubricants and, consequently, improved machines of technological and military importance. The approach is molecular dynamics simulations to provide detailed information about the tribochemistry that occurs when films of carbon solid-state lubricants, such as graphite and diamond-like carbon, are placed between two metal surfaces that are in sliding contact with each other. To facilitate realistic interactions between the covalent carbon atoms and the metal atoms, a combined many-body carbon-metal (MBCM) potential must be constructed that allows one to examine systems composed of thousands of atoms on a standard workstation.

Approach:

A combined many-body carbon-metal (MBCM) potential suitable for use in large-scale atomistic simulations has been constructed. The combined potential reduces to the reactive empirical bond order (REBO) form of Brenner et al. for carbon-carbon and carbon-hydrogen interactions, and to the corrected effective-medium (CEM) form for metal-metal interactions. The metal-carbon interactions are characterized by an expression of the effective-medium type.

Conclusions:

The MBCM potential yields results for test systems that are in good qualitative agreement with available first principles data. Most of the trends are captured correctly, and the potential could be used to study the *general* tribochemistry of a metallic material interacting with a covalently bonded material. It is also expected that the potential will open up to large scale computing many other important problems in materials and surface science, such as corrosion and heterogeneous catalysis. However, some refining will be necessary to obtain improved quantitative agreement with the first principles data and to allow charge transfer between the atoms.

Students and Postdocs funded through the grant:

At this time the PI has two students, Mr. Lifeng Qi and Mr. Matthew Flanagan. They are not supported by the grant directly. However, the grant did allow the PI to purchase most of the equipment needed for the research effort, thus allowing other funds to be used for student support.

Publications, Presentations, Patents and Reports Associated with the Grant:

None.

Transitions that Resulted from the Research:

None.

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